The phase diagram of quantum systems: Heisenberg antiferromagnets

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A novel approach for studying phase transitions in systems with quantum degrees of freedom is discussed. Starting from the microscopic hamiltonian of a quantum model, we first derive a set of exact differential equations for the free energy and the correlation functions describing the effects of fluctuations on the thermodynamics of the system. These equations reproduce the full renormalization group structure in the neighborhood of a critical point keeping, at the same time, full information on the non universal properties of the model. As a concrete application we investigate the phase diagram of a Heisenberg antiferromagnet in a staggered external magnetic field. At long wavelengths the known relationship to the Quantum Non Linear σ Model naturally emerges from our approach. By representing the two point function in an approximate analytical form, we obtain a closed partial differential equation which is then solved numerically. The results in three dimensions are in good agreement with available Quantum Monte Carlo simulations and series expansions. More refined approximations to the general framework presented here and few applications to other models are briefly discussed.

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I. INTRODUCTION

In recent years several works have appeared in the literature on the quantum Heisenberg antiferromagnet, with particular attention to the two dimensional case, because of its deep connections to the physics of high temperature superconductors. Although the corresponding classical model was studied by means of several techniques ranging from high temperature expansions[1] to Monte Carlo (MC) simulations[2] and Renormalization Group (RG)[3] approaches, accurate numerical results on the phase diagram of the quantum model have become available only recently[4,5]. Since the pioneering works based on spin-wave theory[6] and on high-temperature expansions[1], a better understanding of the behavior in two dimensions[7] and of the critical properties in three dimensions[4,8] has been provided by more and more efficient MC methods. Nevertheless, several problems are still open, especially in the low and intermediate temperature region. This regime has been successfully investigated by means of the RG, after an appropriate mapping onto the nonlinear sigma model ($NL\sigma M$)[9]. The satisfactory agreement between RG and experimental results, however, seems to hold only for spin 1/2 and quantitative deviations between theory and experiments[10] appear for larger values of S. Both Monte Carlo simulations[7] and series expansions[11] suggest that the breakdown of the $NL\sigma M$description of a Quantum Antiferromagnet is due to the intrinsic limitations of the methods based on effective actions. In fact, these approaches are devised for describing the long wavelength behavior of the model and can be justified in a regime characterized by strong correlations, while the experimental investigations span a wide temperature range, including regions where local antiferromagnetic order is weak. The same conclusions are also found by use of a new semiclassical approach in which the problem of the quantum Heisenberg antiferromagnet is reduced to a classical one at an effective temperature taking into account quantum fluctuations[12].

Besides the problems concerning the Heisenberg antiferromagnets in bipartite lattices, several other questions are still open in the framework of phase transitions in quantum systems. Generally, accurate analytical approaches at finite temperature are not available and quantum simulations are often hindered by the "sign problem". For instance, frustrated antiferromagnets or fermionic systems, like the celebrated Hubbard model, are still beyond the capabilities of today's simulation algorithms. Interestingly, this class of models might be investigated by a straightforward generalization of the method we are going to present here, at least in order to estimate the magnetic phase boundaries or the occurrence of phase separation.

In this paper, we present a new approach to the phase transitions in quantum systems. A preliminary account can be found in Ref.[13]. We develop a general formalism which can be used in a wide range of temperatures both above and below a possible critical point. The method is then applied to the specific case of Heisenberg antiferromagnets, for different values of the spin and of the spatial dimensions. This approach, which we called QHRT (Quantum Hierarchical Reference Theory) is a quantum extension of the classical HRT which was developed in the context of liquid-vapor transitions and successively applied to several system, like Ising models and binary mixtures[14]. Our method relies on the fact that, for a large class of quantum systems, an exact mapping exists between the quantum

partition function and a fictitious classical one to which HRT can be applied. The main advantage of HRT, also shared by QHRT, is its microscopic character, which allows to obtain both universal and non universal quantities of the system under consideration. Non classical critical exponents together with a precise determination of the critical temperature and a correct description of the first order phase transitions are in fact obtained within the QHRT formalism. As already mentioned, the theory is very general and can in principle be applied to several physical systems, bosons, fermions and spins.

Following the idea of the RG approach, an evolution equation is derived, starting from the perturbative expansion of the Helmholtz free energy. Fluctuations over progressively larger lengthscales are taken into account by varying a cut-off parameter thereby connecting the system with no fluctuations (mean-field approximation) to the fully interacting one. The equation obtained in this way is formally exact, although it is not written in a closed form. In order to get a closed equation, the knowledge of the structure of the dynamic correlation functions of the model as a function of frequency and wavevector is needed. This represents the only approximation present in the QHRT approach and requires a thorough analysis of its physical implications. Near a critical point our partial differential equation acquires a universal form and reproduces the RG structure for a three component order parameter with critical exponents exact to first order in $\epsilon = 4 - d$. Also as $T \to 0$, the QHRT approach is able to predict the known behavior originally derived by a RG analysis of the $NL\sigma M$. We solved the equation for several values of the spin, both in two and three spatial dimensions. In $d = 3$ we obtained an excellent matching with the available numerical simulation data, also from a quantitative point of view.

The paper is organized as follows: In Section II we give the derivation of the theory. In Section III the theory is applied to the Heisenberg antiferromagnets, the classical Heisenberg model being obtained as the limiting $S \to \infty$ case. In Section IV an explicit closure is given and the implications of this choice are discussed. In Section V an analysis of QHRT equation in proximity of a phase transition is given. In Section VI the explicit results, obtained via numerical integration of the evolution equation, are presented. Finally in Section VII conclusions are drawn and further possible applications of our theory are proposed.

II. DERIVATION OF QHRT EQUATIONS

In this Section we develop a general formalism for the description of critical phenomena in quantum systems. Our goal is to implement the basic ideas of renormalization group to the microscopic, many body hamiltonian of an interacting quantum model. The class of hamiltonians we are going to consider, in arbitrary dimension d, has the structure:

$$\hat{H} = \hat{H}_R + \hat{V} = \hat{H}_R + \frac{1}{2}\int dxdy\hat{\rho}(x)w(x-y)\hat{\rho}(y) \tag{1}$$

where $\hat{H}_R$ is a reference part whose properties are supposed known and the coordinates x and y span the d-dimensional space. $\hat{V}$ represents an interaction term which couples the (local) observables $\hat{\rho}(r)$ at two different points via the translationally invariant two body potential $w(x-y)$. In the following we will assume that: i) the local operators $\hat{\rho}(r)$ commute at different points and ii) the interaction $w(r)$ can be Fourier transformed. Instead, no limitation is imposed on the form of $\hat{H}_R$, which is *not* restricted to describe free particles. This class of hamiltonians is indeed rather general and includes several systems of widespread interest, like quantum magnets (where $\hat{\rho}(r)$ represents a spin variable) but also models of interacting fermions, both on and off lattice (where $\hat{\rho}(r)$ is the local density operator) and even systems with electron-phonon coupling, like the Hubbard-Holstein model. Generalizations to other cases, for instance models with many particle interactions, are possible but will not be considered here.

As a first step, we will write the partition function of the quantum model in a form identical to that of a classical system. The latter will be then studied by means of the powerful methods already available in the framework of classical critical phenomena. This *quantum to classical* mapping is most easily carried out by expanding the grand canonical partition function Ξ as a power series of $w(r)$. The method we use closely follows the standard treatment of the path integral formulation of quantum mechanics[15], although we carefully avoid to introduce any smoothness assumption on the classical fields. Therefore, our treatment is *not* limited to long wavelength or low energy and the equations we are going to obtain are formally exact in the whole phase diagram of the model.

The grand partition function of the quantum system, $\Xi = \mathrm{Tr}\,\exp(-\beta\hat{H})$, is first written in terms of the (imaginary time) evolution operator[16] as:

$$\mathrm{Tr}\,\exp(-\beta\hat{H}) = \mathrm{Tr}\left\{\exp(-\beta\hat{H}_R)\hat{U}(\beta)\right\} \tag{2}$$

where $\hat{U}(t)$ is the solution of the differential equation:

$$\frac{d}{dt}\hat{U}(t) = -\hat{V}(t)\hat{U}(t) \tag{3}$$

with $\hat{U}(0) = 1$ as initial condition. $\hat{V}(t)$ is the time dependent operator:

$$\hat{V}(t) = \exp[\hat{H}_R t]\, \hat{V}\, \exp[-\hat{H}_R t] \tag{4}$$

Equation (3) can be formally solved by iteration with the result:

$$\hat{U}(t) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^t dt_1 ... \int_0^t dt_n T_t[\hat{V}(t_1)...\hat{V}(t_n)] \tag{5}$$

where T_t is the usual time ordering operator. By inserting in (5) the explicit form of $\hat{V}(t)$

$$\hat{V}(t) = \frac{1}{2} \int dxdy \int dt' \hat{\rho}(x,t) w(x-y) \delta(t-t') \hat{\rho}(y,t') \tag{6}$$

equation (2) can be written as a power series of the $(d+1)$-dimensional interaction

$$\phi(X, X') = w(x-x')\delta(t-t') \tag{7}$$

Here, the variable X identifies the pair (x,t) where x spans the d-dimensional coordinate space and t belongs to the interval $(0,\beta)$. The explicit expression for the grand partition function Ξ is:

$$\begin{aligned} \Xi &= \mathrm{Tr}\, e^{-\beta \hat{H}} \\ &= \Xi_R \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n\, n!} \int dX_1 dX_1' ... dX_n dX_n'\, \rho_R(X_1, ...X_n')\, \phi(X_1, X_1') ... \phi(X_n, X_n') \end{aligned} \tag{8}$$

Here and in the following R labels the reference system defined by $\hat{H}_R$. The imaginary time dynamic correlation functions appearing in Eq. (8) $\rho(X_1, ...X_n)$ are defined, for a general hamiltonian $\hat{H}$, by:

$$\rho(x_1, t_1; ...x_n, t_n) = \langle \hat{\rho}(x_1, t_1) ... \hat{\rho}(x_n, t_n) \rangle = \frac{1}{\Xi} \mathrm{Tr} \left\{ e^{-\beta \hat{H}}\, T_t[\hat{\rho}(x_1, t_1) ... \hat{\rho}(x_n, t_n)] \right\} \tag{9}$$

where $\hat{\rho}(x,t)$ is the local density operator in imaginary time:

$$\hat{\rho}(x,t) = \exp[\hat{H}t]\, \hat{\rho}(x)\, \exp[-\hat{H}t] \tag{10}$$

The correlation functions in the perturbative expansion (8) are given by Eqs. (9,10) specialized to the reference hamiltonian $\hat{H}_R$. Since $\hat{\rho}(r)$ commutes on different sites, the functions (9) are symmetric under the permutation of the labels and can be viewed as the correlation functions of a hypothetical $(d+1)$ dimensional *classical* reference system. The quantum nature of the problem is then contained in the structure of the reference system through Ξ_R and $\rho_R(X_1, ...X_n)$. It is interesting to notice that the n-particle correlation functions $\rho(X_1, ...X_n)$ associated to a given quantum hamiltonian $\hat{H}$ can be equivalently obtained as successive functional derivatives of a generalized partition function $\Xi[J]$ with respect to a space and time dependent external field $J(x,t)$ coupled to the quantum operator $\hat{\rho}(x)$. More precisely, the generating functional $\Xi[J]$ is still defined as the trace of an imaginary time evolution operator:

$$\Xi[J] = \mathrm{Tr} \left\{ \exp[-\beta \hat{H}] \hat{U}(\beta) \right\} \tag{11}$$

where now $\hat{U}(t)$ is the solution of the differential equation:

$$\frac{d}{dt}\hat{U}(t) = -\hat{K}(t)\hat{U}(t) \tag{12}$$

with initial condition $\hat{U}(0) = 1$ and

$$\hat{K}(t) = -\int dx J(x,t) \hat{\rho}(x,t) \tag{13}$$

Following the same steps which led to Eq. (8) it is easy to show that the correlation functions $\rho(x_1,t_1;...x_n,t_n)$ generated by $\Xi[J]$

$$\rho(x_1,t_1;...x_n,t_n) = \frac{1}{\Xi[J]} \left. \frac{\delta^n \Xi[J]}{\delta J(x_1,t_1)...\delta J(x_n,t_n)} \right|_{J=0} \tag{14}$$

reduce to those defined in (9). Analogously, it is useful to introduce the connected correlation functions defined by:

$$F(x_1,t_1;...x_n,t_n) = \left. \frac{\delta^n \ln \Xi[J]}{\delta J(x_1,t_1)...\delta J(x_n,t_n)} \right|_{J=0} \tag{15}$$

In the following, we will take the perturbative expansion (8) as a definition of the fully interacting partition function where the reference n-particle correlation functions are written as functional derivatives via Eqs. (14,15). Now the quantum to classical correspondence is complete: Having defined the (quantum) reference system by a hamiltonian $\hat{H}_R$, we compute the corresponding functional $\Xi_R[J]$ via Eq. (11). If we interpret this quantity as the grand partition function of a fictitious classical reference system in $d+1$ dimensions in an external field $J(x,t)$ coupled to a scalar order parameter $\psi(x,t)$ and at an effective temperature $T_{cl}=1$, the exact partition function of the quantum system (8) formally coincides with that of such a classical system with the additional non local coupling (7) in the field $\psi(x,t)$ at two different space-time points.

For future reference, let us briefly discuss the general relationship between the previously introduced imaginary time two point function (14) and the physically relevant dynamic correlations defined by:

$$D(x_1-x_2,t_1-t_2) = \frac{i}{\Xi} \mathrm{Tr} \left\{ e^{-\beta \hat{H}} e^{i\hat{H}t_1} \Delta\hat{\rho}(x_1) e^{-i\hat{H}t_1} e^{i\hat{H}t_2} \Delta\hat{\rho}(x_2) e^{-i\hat{H}t_2} \right\} \tag{16}$$

where $\Delta\hat{\rho}(x) = \hat{\rho}(x) - <\hat{\rho}(x)>$. Taking the Fourier transform in the space and time variables and inserting a complete set of basis states we get the usual Lehmann representation for the spectral function:

$$\mathrm{Im}\, D(k,\omega) = \frac{2\pi}{\Xi} \sum_{s,s'} e^{-\beta E_s} |< s|\hat{\rho}_k|s'>|^2 \delta(\omega - E_{s'} + E_s) \tag{17}$$

which obeys the detailed balance relation $\mathrm{Im}\, D(k,\omega) = \mathrm{Im}\, D(-k,-\omega)\exp(\beta\omega)$. The analogous expression for the imaginary time correlation function reads:

$$F(k,\omega_n) = \frac{1}{\Xi} \sum_{s,s'} \frac{e^{-\beta E_s} - e^{-\beta E_{s'}}}{E_{s'} - E_s - i\omega_n} |< s|\hat{\rho}_k|s'>|^2 \tag{18}$$

where we took advantage of the periodicity of the two particle correlation function (9) in the imaginary time variable $t = t_1 - t_2$ with period β. As a consequence, the frequency variable ω_n is now an integer multiple of $2\pi/\beta$. By comparing Eqs. (17) and (18) we get the final relation, valid for systems with inversion symmetry:

$$F(k,\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \mathrm{Im}\, D(k,\omega) \frac{\omega}{\omega^2+\omega_n^2} \qquad \text{for } \omega_n \neq 0 \tag{19}$$

This equation will be useful in order to relate the correlation function $F(k,\omega)$ to physical observables.

In order to derive a set of renormalization group equations for the model hamiltonian (1), we follow the same strategy successfully adopted in classical systems[14]: First we obtain a formal expansion of the Helmholtz free energy of the quantum model in powers of the two body interaction $w(x)$. Then we define a sequence of intermediate systems (*Q-systems*) in which fluctuations characterized by wavevectors $k<Q$ are inhibited. Finally we write a differential equation for the "evolution" of the free energy when the infrared cut-off Q is changed by an infinitesimal amount. Analogously to the classical case, the resulting equation is exact but cannot be written in closed form because it involves the knowledge of the two particle correlation function of the Q-systems. In fact, this is only the first equation of an infinite hierarchy of differential equations for the free energy and n-particle correlation function of the model, which form the Quantum Hierarchical Reference Theory of Fluids (QHRT).

Let us briefly sketch the basic steps necessary to derive the first QHRT equation: Details can be found in Ref.[14] via the quantum to classical correspondence previously discussed. The perturbative expansion of the logarithm of the grand partition function is directly obtained from Eq. (8) in terms of the connected correlation functions (15) of the reference system, denoted by F_R. Next we perform a Legendre transformation which defines the Helmholtz free

energy $A[\rho]$ as a functional of the order parameter profile $\rho(x) = \beta^{-1}\left(\delta \ln \Xi / \delta J(x)\right)$ corresponding to a static external field $J(x)$:

$$A[\rho] = -\beta^{-1} \ln \Xi[J] + \int dx J(x)\rho(x) \tag{20}$$

The perturbation series of the free energy in powers of the interaction is then given by a diagrammatic expansion involving the pair potential (7) and the reference correlation functions (15). This series can be conveniently ordered according to the number of loops: the terms up to the one loop level reproduce the well known random phase approximation (RPA) to the free energy of the interacting system. In the homogeneous limit $\rho(x) = \rho$, the expansion reads:

$$A = A_R + \frac{1}{2} V \rho^2 \tilde{w}(k=0) - \frac{1}{2} V \rho w(r=0) + V \frac{1}{2\beta} \sum_{\omega_n} \int \frac{d^d k}{(2\pi)^d} \ln\left[1 + F_R(k,\omega_n)\tilde{w}(k)\right] + \mathcal{L}_2 \tag{21}$$

Here V is the volume of the system, $\mathcal{L}_2$ represents the sum of all the diagrams with at least two loops, whose structure we do not need to detail, k is the wavevector and $\omega_n = 2\pi n/\beta$ are the usual Matsubara frequencies coming from the Fourier transform in the imaginary time direction, while $\tilde{w}(k)$ is the Fourier transform of the two body interaction $w(x)$.

Now we define a sequence of Q-systems interpolating between the reference system and the fully interacting one by introducing a cut-off Q in the wavevector integration of every loop of the expansion (21). Clearly, for $Q \to 0$ we recover the full expansion (21) to all orders while for $Q \to \infty$ all contributions to the free energy with at least one loop are suppressed and we get the mean field expression for the Helmholtz free energy:

$$A_{Q=\infty} = A_R + \frac{1}{2} V \rho^2 \tilde{w}(k=0) - \frac{1}{2} V \rho w(r=0) \tag{22}$$

Analogously, the two point function $F(k,\omega_n)$ admits a perturbative expansion in powers of $w(r)$ which can be again ordered according to the number of loops. Only the zero loop (chain) terms survive in the $Q \to \infty$ limit reproducing the well known RPA result:

$$F_{Q=\infty}(k,\omega_n) = \frac{F_R(k,\omega_n)}{1 + F_R(k,\omega_n)\tilde{w}(k)} \tag{23}$$

These results show that, through the sequence of Q-systems, thermal and quantum fluctuations are gradually turned on and consequently, the free energy of the Q-system continuously connects the mean field approximation (22,23) to the exact expression corresponding to the fully interacting model.

As already noticed for the classical case[14], it is possible to write an exact differential equation describing the Q-evolution of the free energy A_Q. The key observation is that in all the diagrams of the expansion (21), including the terms collectively named $\mathcal{L}_2$, every loop contains at least an interaction bond. Therefore, limiting each momentum integration to the domain $k > Q$ can be equally achieved by cutting off the Fourier components of the interaction $\tilde{w}(k)$ at small momenta. Then, the Q-system can be equivalently defined as the system interacting via the pair potential:

$$\tilde{w}_Q(k) = \begin{cases} \tilde{w}(k) & \text{if } k > Q \\ 0 & \text{if } k < Q \end{cases} \tag{24}$$

The only *caveat* concerns the zero loop diagrams in the diagrammatic expansion of the free energy, which only depend on the zero momentum component of the perturbation potential $\tilde{w}_Q(k)$. According to the definition (24), $\tilde{w}_Q(k=0)$ identically vanishes for every $Q \neq 0$: The zero loop contributions are then absent from the free energy corresponding to the potential (24), while were included in the previous definition of Q-system. Therefore, in order to get the free energy of the Q-system from the free energy of the hypothetical model interacting through the potential w_Q, we must explicitly add the zero loop contributions, which have been already evaluated in Eq. (22). Similar considerations hold for the two point function of the Q-system $F_Q(k)$ which differs from that corresponding to the interaction w_Q because of the simply connected (chain) diagrams. However, these terms are proportional to the k^{th} Fourier component of the interaction $\tilde{w}_Q(k)$ which, according to the definition (24), coincides with $\tilde{w}(k)$ for every $k > Q$ while vanishes if $k < Q$. Therefore, the chain contribution needs to be added to the two particle correlation function of the system with interaction w_Q only for $k < Q$. As a consequence, the two point function of the model with interaction w_Q, which we denote by $\hat{F}_Q(k,\omega_n)$ is discontinuous in k space on the $k = Q$ surface and can be expressed in terms of the two point function of the Q-system $F_Q(k)$ as

$$\hat{F}_Q(k,\omega_n) = \begin{cases} F_Q(k,\omega_n) & \text{if } k > Q \\ \dfrac{F_Q(k,\omega_n)}{1 - F_Q(k,\omega_n)\tilde{w}(k)} & \text{if } k < Q \end{cases} \tag{25}$$

This one to one correspondence between Q-systems and models interacting via the potential (24) is extremely useful in order to obtain the QHRT evolution equations. According to the previous discussion, the change in the free energy of the Q-system corresponding to a change in the cut-off $Q \to Q - \delta Q$ can be evaluated by means of the perturbative expansion (21) in which the "reference" free energy is now identified as A_Q and the perturbation potential as $[\tilde{w}_{Q-\delta Q}(r) - \tilde{w}_Q(r)]$. Such a potential has Fourier components only in the infinitesimal momentum shell defined by $Q - \delta Q < k < Q$. In the limit $\delta Q \to 0$, by keeping only terms $O(\delta Q)$ we just select the one loop diagrams which have been explicitly summed up in Eq. (21), while all the many loop contributions $\mathcal{L}_2$ are at least of order $(\delta Q)^2$, i.e. rigorously negligible. The zero loop terms are trivial and have been automatically included form the beginning through the initial condition (22). The resulting differential equation for the evolution of the free energy density is then:

$$\frac{d}{dQ}\left(\frac{A_Q}{V}\right) = \frac{Q^{d-1}}{2\beta} \sum_{\omega_n} \int_{k=Q} \frac{d\Omega_k}{(2\pi)^d} \ln[1 - F_Q(k,\omega_n)\tilde{w}(k)] \tag{26}$$

where the momentum integral is limited on the shell $k = Q$ and then reduces to the integration over the solid angle Ω_k.

This evolution equation is exact and must be supplemented by the initial condition (22) at $Q = \infty$. However, the presence of the two point function $F_Q(k,\omega_n)$ at right hand side prevents the possibility to obtain the thermodynamics of the model without introducing some sort of approximation. In the following we will discuss a closure to Eq. (26) based on a parametrized form of the two point function which is related by an exact sum rule to the Helmholtz free energy A_Q of the Q-system. The justification of this closure relation requires, however, an analysis of the physical properties of the model we want to investigate and therefore we first have to specialize this rather general presentation of the QHRT equations to the case of the antiferromagnetic Heisenberg model which will be thoroughly investigated in the following Sections.

III. QHRT EQUATION FOR THE ISOTROPIC HEISENBERG MODEL

In this Section, the QHRT formalism just developed will be applied to the study of the isotropic antiferromagnetic Heisenberg model on a N-site cubic lattice in arbitrary dimension d and spin S. This is an extremely interesting many body model which allows to study the interplay of thermal and quantum fluctuations in determining the phase diagram of the system and the effects of spatial dimensionality on the occurrence of long range order[17]. In the $S \to \infty$ limit, quantum fluctuations are suppressed and the system behaves classically. This regime has been extensively studied by series expansions[1], numerical simulations[2], renormalization group techniques[3] and approximate theoretical approaches[18]. Much less is known at finite values of the local spin S: accurate simulations have become available only recently while series expansions are known to lose accuracy both at low temperature and in the critical region.

Since we want to investigate the paramagnetic-antiferromagnetic transition, it is convenient to consider the presence of an external magnetic field h, parallel to the z axis, which couples to the order parameter, i.e. to the staggered magnetization:

$$\hat{H} = J \sum_{<\mathbf{R},\mathbf{R}'>} \hat{\mathbf{S}}_{\mathbf{R}} \cdot \hat{\mathbf{S}}_{\mathbf{R}'} - h \sum_{\mathbf{R}} e^{i\mathbf{g}\cdot\mathbf{R}} \hat{S}^z_{\mathbf{R}} \tag{27}$$

Here $J > 0$, $\mathbf{g}$ is the antiferromagnetic wavevector of components $g_i = \pi$, while the spin operators $\hat{\mathbf{S}}$ satisfy the usual commutation relations

$$\left[\hat{S}^i_{\mathbf{R}}, \hat{S}^j_{\mathbf{R}'}\right] = i\delta_{\mathbf{R},\mathbf{R}'}\epsilon_{i\,j\,k}\hat{S}^k_{\mathbf{R}} \tag{28}$$

The lower and upper indices label respectively the site on the lattice and the component of the spin, while $\epsilon_{i\,j\,k}$ is the totally antisymmetric tensor. With respect to the class of hamiltonians examined in the previous Section, the Heisenberg model requires some straightforward extension because i) the system is defined on a lattice, which is not isotropic; ii) the order parameter is now the staggered magnetization: a three component vector. As a consequence,

the correlation functions acquire spin component indices and *iii*) the presence of a staggered magnetic field breaks translation invariance by one lattice site.

The reference system is chosen to be defined by the non interacting hamiltonian

$$\hat{H}_R = -h \sum_{\mathbf{R}} e^{i\mathbf{g}\cdot\mathbf{R}} \hat{S}^z_{\mathbf{R}} \tag{29}$$

whose properties can be easily obtained. For instance, the grand potential as a function of the number of sites N, inverse temperature β and staggered field h reads:

$$\log \Xi_R = N \ln \left[\sinh(\beta h S) \coth(\beta h/2) + \cosh(\beta h S) \right] \tag{30}$$

The staggered magnetization m can be found by differentiating (30) with respect to βh and the Helmholtz free energy then follows by Legendre transform (20). However, the explicit inversion formulae can be found analytically only in the $S = 1/2$ case where

$$\begin{aligned} \beta A_R &= N \left[(\frac{1}{2} + m) \ln(\frac{1}{2} + m) + (\frac{1}{2} - m) \ln(\frac{1}{2} - m) \right] \\ \beta h &= \ln \left[\frac{\frac{1}{2} + m}{\frac{1}{2} - m} \right] \end{aligned} \tag{31}$$

In order to derive the renormalization group equation appropriate for the magnetic transition in this model, we now have to suitably define the sequence of Q-systems whose role is to gradually introduce fluctuations into the system. The critical fluctuations occur at a wavevector $\mathbf{k} = \mathbf{g}$ and then it is natural to define a sequence of systems in which the Fourier components of the potential $\tilde{w}(\mathbf{k})$

$$\tilde{w}(\mathbf{k}) = 2J\gamma(\mathbf{k}) \qquad\qquad \gamma(\mathbf{k}) = \sum_{i=1}^{d} \cos k_i \tag{32}$$

are suppressed in a neighborhood of $\mathbf{k} = \mathbf{g}$. A convenient choice is to limit the domain of integration in $\mathbf{k}$ space by

$$|\gamma(\mathbf{k})| < \sqrt{d^2 - Q^2} \tag{33}$$

with $Q \in (0, d)$. As $Q \to 0$ all Fourier components are included and we recover the fully interacting system. At $Q = d$ the free energy density $a = A/N$ includes only the reference term and the zero loop contribution:

$$a_{Q=d} = a_R - dJm^2 \tag{34}$$

The two particle correlation function is represented by a a 3×3 matrix which, due to the spin symmetries in the Hamiltonian under rotations around the z axis, has the following general structure in Fourier space:

$$F = \begin{pmatrix} F^{xx} & F^{xy} & 0 \\ F^{yx} & F^{yy} & 0 \\ 0 & 0 & F^{zz} \end{pmatrix} \tag{35}$$

The three independent entries are given by:

$$\begin{aligned} F^{xx}(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2) &= F^{yy}(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2) = F^{xx}(\mathbf{k}_1, \omega_1)\, \beta\, N \delta(\omega_1 + \omega_2)\, \delta(\mathbf{k}_1 + \mathbf{k}_2) \\ F^{xy}(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2) &= -F^{yx}(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2) = F^{xy}(\mathbf{k}_1, \omega_1)\, \beta\, N \delta(\omega_1 + \omega_2) \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{g}) \\ F^{zz}(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2) &= F^{zz}(\mathbf{k}_1, \omega_1)\, \beta\, N \delta(\omega_1 + \omega_2)\, \delta(\mathbf{k}_1 + \mathbf{k}_2) \end{aligned} \tag{36}$$

where $\mathbf{k}$ belongs to the first Brillouin zone and ω is an integer multiple of $2\pi/\beta$. Because of the presence of the external field, the translational invariance is broken and the two point function is not proportional to $\delta(\mathbf{k}_1 + \mathbf{k}_2)$. Nevertheless,

due to the symmetry of the hamiltonian under a translation of one lattice site and a simultaneous rotation of π around x axis, the diagonal elements and the off-diagonal elements are respectively proportional to $\delta(\mathbf{k}_1+\mathbf{k}_2)$ and to $\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{g})$ as stated in Eq. (36). At $Q=d$, the summation of the zero loop diagrams explicitly gives:

$$F^{xx}_{Q=d}(\mathbf{k},\omega) = \frac{\mu_\perp - \tilde{w}(\mathbf{k})}{m^{-2}\omega^2+\mu_\perp^2-\tilde{w}(\mathbf{k})^2}$$

$$F^{xy}_{Q=d}(\mathbf{k},\omega) = \frac{m^{-1}\omega}{m^{-2}\omega^2+\mu_\perp^2-\tilde{w}(\mathbf{k})^2}$$

$$F^{zz}_{Q=d}(\mathbf{k},\omega) = \frac{\delta_{\omega,0}}{\mu_{||}+\tilde{w}(\mathbf{k})} \tag{37}$$

where $\mu_\perp$ and $\mu_{||}$ are functions of temperature and staggered magnetization m given, for $S=1/2$, by:

$$\beta\mu_\perp = 2m^{-1}\tanh^{-1}(2m) \qquad\qquad \beta\mu_{||} = 4(1-4m^2)^{-1} \tag{38}$$

Having determined the mean field form (i.e the zero loop contribution) of the relevant quantities, we now turn to the inclusion of fluctuations via the definition of the QHRT renormalization group equation. Following the procedure outlined in the previous Section and taking into account the definition (33) of Q-systems, we find the exact evolution equation for the free energy density $a_Q = A_Q/N$ of the antifferromagnetic Heisenberg model which should be solved with the appropriate initial condition (34) at $Q=d$:

$$\frac{d\,a_Q}{dQ} = \frac{1}{2\beta}\sum_{\omega_n}\int \frac{d^dk}{(2\pi)^d}\,\delta(\sqrt{d^2-\gamma(\mathbf{k})^2}-Q)\Big\{\ln(1-F^{zz}_Q(\mathbf{k},\omega_n)\tilde{w}(\mathbf{k}))+ \tag{39}$$

$$\ln\Big[(1-F^{xx}_Q(\mathbf{k},\omega_n)\tilde{w}(\mathbf{k}))(1+F^{xx}_Q(\mathbf{k}+\mathbf{g},\omega_n)\tilde{w}(\mathbf{k})) - F^{xy}_Q(\mathbf{k},\omega_n)F^{xy}_Q(\mathbf{k}+\mathbf{g},\omega_n)\tilde{w}(\mathbf{k})^2\Big]\Big\}$$

The summation of the one loop (ring) diagrams, necessary to obtain Eq (39), must be carried out by carefully exploiting the frequency and momentum conservation rules (36). The delta function present in the d-dimensional integral (39) limits the integration domain to the surface Σ_Q defined by $\gamma(\mathbf{k}) = \pm\sqrt{d^2-Q^2}$. This equation, although formally exact, is not closed because the evolution of the free energy depends on the unknown magnetic structure factors of the model $F^{ij}_Q(\mathbf{k},\omega)$ at a generic value of the cut-off Q while these quantities are known only at the beginning of the integration, i.e. at $Q=d$ where they have the form shown in Eq. (37). If we simply assume that $F^{ij}_Q(\mathbf{k},\omega)$ is not affected by fluctuations, the QHRT equation reproduces the the standard RPA approximation. A better treatment of fluctuations needs a more flexible parameterization of the correlation functions. This delicate point requires a detailed analysis of the properties of the (imaginary time) dynamic structure factors of the Heisenberg model, which will be carried out in the next Section.

IV. TWO BODY CORRELATIONS

In this Section we exploit some known feature of quantum antiferromagnets in order to derive constraints on the formal structure of the two point functions $F^{ij}_Q(\mathbf{k},\omega_n)$ required to close the QHRT evolution equation (39).
As a first step, let us recall the relationship between the dynamic correlations of the Heisenberg model, defined in physical frequency, and the imaginary time functions which enter the QHRT formalism. The general correspondence has been already obtained in Eq. (19): Here we point out that the analytical form of the mean field correlation functions (37), which serves as initial condition, reproduces the single mode approximation in the dynamic structure factor:

$$\begin{aligned}\mathrm{Im}\,S^{xx}(\mathbf{k},\omega) &= \frac{\pi\omega}{1-\exp(-\beta\omega)}\frac{\delta(\omega-\epsilon_k)+\delta(\omega+\epsilon_k)}{\mu_\perp+\tilde{w}(\mathbf{k})}\\ \mathrm{Im}\,S^{zz}(\mathbf{k},\omega) &= \frac{2\pi}{\beta}\,\frac{\delta(\omega)}{\mu_{||}+\tilde{w}(\mathbf{k})}\end{aligned} \tag{40}$$

where

$$\epsilon_k = m\sqrt{\mu_\perp^2-\tilde{w}(\mathbf{k})^2} \tag{41}$$

can be recognized as the dispersion relation for spin waves in this approximation. The elastic sum rule immediately gives the corresponding form of the equal time structure factor via integration over the frequency axis:

$$S_\perp(\mathbf{k}) = \frac{1}{\beta}\sum_{\omega_n} F^{xx}(\mathbf{k},\omega_n) = \frac{\epsilon_k}{2\tanh(\beta\epsilon_k/2)}\,\frac{1}{\mu_\perp + \tilde{w}(\mathbf{k})}$$
$$S_{||}(\mathbf{k}) = \frac{1}{\beta}\sum_{\omega_n} F^{zz}(\mathbf{k},\omega_n) = \frac{1}{\beta}\frac{1}{\mu_{||} + \tilde{w}(\mathbf{k})} \tag{42}$$

These expressions show that both the dynamic and static structure factors (40,42) coincide with those usually adopted in the interpretation of neutron scattering data, in the limit of negligible spin wave damping[19]. This suggests that the simple analytical structure of Eqs. (37) qualifies as a good starting point for obtaining a closure relation to the QHRT equation. However, the parameters $\mu_\perp$ and $\mu_{||}$ appearing in the correlation functions (37) will be modified by fluctuations and cannot be identified with their mean field estimate (38) down to $Q = 0$. These quantities can be directly related to important physical properties of the model: The definition (15) of n-point function shows that the zero frequency value of $F^{ii}(\mathbf{k},\omega_n)$ coincides with the uniform (staggered) susceptibility χ° (χ^s) when $\mathbf{k} = 0$ ($\mathbf{k} = \mathbf{g}$) and therefore

$$\chi^\circ_\perp = F^{xx}(0,0) = (\mu_\perp + 2Jd)^{-1}$$
$$\chi^\circ_{||} = F^{zz}(0,0) = (\mu_{||} + 2Jd)^{-1} \tag{43}$$
$$\chi^s_\perp = \left(\frac{h}{m}\right)^{-1} = m\left(\frac{\partial a}{\partial m}\right)^{-1} = F^{xx}(\mathbf{g},0) = (\mu_\perp - 2Jd)^{-1}$$
$$\chi^s_{||} = \left(\frac{\partial h}{\partial m}\right)^{-1} = \left(\frac{\partial^2 a}{\partial m^2}\right)^{-1} = F^{zz}(\mathbf{g},0) = (\mu_{||} - 2Jd)^{-1} \tag{44}$$

Here, we have conveniently expressed the staggered susceptibilities as thermodynamic derivatives of the external field h and of the free energy density a with respect to the staggered magnetization m, using the isotropy of the model in the spin variables. At the critical point and in the whole coexistence region, both the longitudinal and the transverse susceptibilities diverge[3], implying that $\mu_\perp = \mu_{||} = 2Jd$. This feature leads to a gapless spin wave spectrum, via Eq. (41), with linear behavior near $\mathbf{k} = 0$ (and $\mathbf{k} = \mathbf{g}$): $\epsilon_k \sim c_s k$. In the approximation (37), the associated spin velocity is proportional to the spontaneous staggered magnetization: $c_s = Jm\sqrt{4d}$. At zero temperature, the static transverse structure factor (42) is linear in k around $\mathbf{k} = 0$ in the symmetry broken phase and the prefactor defines the spin stiffness ρ_s[20]:

$$S_\perp(k) \sim \frac{\rho_s}{2c_s}k \tag{45}$$

Within a parameterization of the form (37), the stiffness can be expressed in terms of the spin velocity: $\rho_s = c_s^2/(4Jd) = Jm^2$. Remarkably, the hydrodynamic relation $\chi^\circ_\perp c_s^2 = \rho_s$, which is believed to hold at zero temperature, is satisfied even in this simple approximation.

A known sum rule which is worth mentioning regards the on site value of the static structure factors, which is bound by the spin normalization condition:

$$\frac{1}{\beta}\sum_{\omega_n}\int\frac{d^dk}{(2\pi)^d}\left[F^{zz}(\mathbf{k},\omega_n) + 2F^{xx}(\mathbf{k},\omega_n)\right] + m^2 = S(S+1) \tag{46}$$

at any temperature. If we choose to determine the parameters $\mu_\perp$ and $\mu_{||}$ by use of the susceptibility sum rules (44), in close analogy with the procedure adopted for classical models[14], the additional relation (46) cannot be generally satisfied by the simple form (37). This deficiency is due to the presence of an incoherent part in the actual dynamic correlations which has been neglected in our single mode approximation.

A useful check on the accuracy of the parameterization (37) comes from the zero temperature limit, where quantitative approximations are available, like Spin Wave Theory (SWT). Although SWT is formally an expansion around the classical limit, even the simplest truncations in the parameter $1/S$ are known to be quite accurate even for $S = 1/2$[7]. To lowest order, the spontaneous staggered magnetization attains its maximum value $m = S$ and the correlation functions in imaginary time can be easily calculated in vanishing external field h: Remarkably, the result has precisely the mean field structure (37) with $\mu_\perp = \mu_{||} = 2Jd$, as expected in the symmetry broken state. However, it is known that quantum fluctuations affect the zero field magnetization, the spin wave spectrum ϵ_k, the stiffness ρ_s and the

uniform susceptibility $\chi^{\circ}_{\perp}$. These quantities are indeed modified to first order in SWT[21], although the form of ϵ_k (41) remains unaltered and only the prefactor is changed, leading to a simple renormalization of the spin wave velocity c_s:

$$\begin{aligned} c_s &= Z_c\, JS\sqrt{4d}\,;\; Z_c = 1 + \frac{1}{2S}\int \frac{d^dk}{(2\pi)^d}\,[1-\epsilon_{sw}(\mathbf{k})] \\ \rho_s &= \quad Z_\rho\, JS^2\,; \quad Z_\rho = 1 - \frac{1}{2S}\int \frac{d^dk}{(2\pi)^d}\,\frac{[1-\epsilon_{sw}(\mathbf{k})]^2}{\epsilon_{sw}(\mathbf{k})} \\ \chi^{\circ}_{\perp} &= Z_\chi (J4d)^{-1}\,; Z_\chi = 1 - \frac{1}{2S}\int \frac{d^dk}{(2\pi)^d}\,\frac{1-\epsilon_{sw}(\mathbf{k})^2}{\epsilon_{sw}(\mathbf{k})} \end{aligned} \tag{47}$$

where the momentum integrals are restricted to the lattice Brillouin zone and

$$\epsilon_{sw}(\mathbf{k}) = \sqrt{1 - d^{-2}\gamma^2_{\mathbf{k}}} \tag{48}$$

A better representation of the dynamic correlations which, keeping the single pole structure (40), is able to reproduce the first order SWT results (47) can be obtained by including two more adjustable renormalization amplitudes ζ in the functions $F^{ij}(\mathbf{k},\omega_n)$:

$$\begin{aligned} F^{xx}(\mathbf{k},\omega) &= \zeta_\perp \frac{\mu_\perp - \tilde{w}(\mathbf{k})}{m^{-2}\zeta^2_\perp\omega^2 + \mu^2_\perp - \tilde{w}(\mathbf{k})^2} \\ F^{xy}(\mathbf{k},\omega) &= \zeta_\perp \frac{\zeta_\perp m^{-1}\omega}{m^{-2}\zeta^2_\perp\omega^2 + \mu^2_\perp - \tilde{w}(\mathbf{k})^2} \\ F^{zz}(\mathbf{k},\omega) &= \zeta_{||} \frac{\delta_{\omega,0}}{\mu_{||} + \tilde{w}(\mathbf{k})} \end{aligned} \tag{49}$$

At zero temperature, the full one loop SWT corrections (47) are reproduced by the form (49) with the choice $\zeta_\perp = Z_\chi$ showing that such an ansatz for the dynamic correlation functions may improve the simple mean field description of Heisenberg antiferromagnets. However, in order to implement this generalization we need additional sum rules for determining self-consistently the parameters $\zeta_\perp$ and $\zeta_{||}$, besides the already mentioned Eqs. (44) for $\mu_\perp$ and $\mu_{||}$. A natural choice would be the analogous Eqs. (43), which control the renormalization of the uniform susceptibility. However, we will not explicitly pursue this extension in the present work, but rather confine our analysis to the simplest choice $\zeta_\perp = \zeta_{||} = 1$, i.e. keeping the same structure of the dynamic correlations at the mean field level (37), just allowing for "mass renormalization", according to Eqs. (44). The single mode structure of the dynamic correlations, besides reproducing the lowest order spin wave result at $T = 0$, has also been proven quite accurate in numerical studies on the Heisenberg model both via series expansions[22] and Monte Carlo simulations[4].

As noticed by Hertz in his pioneering work on phase transitions in quantum systems[23], a proper treatment of critical phenomena in quantum mechanics directly provides predictions on dynamic scaling in the system. The same feature is clearly present in our microscopic approach which requires the form of the dynamic structure factor. Unfortunately, in the approximation we are examining, the single pole form (40) does not allow for anomalous scaling in the dispersion relation ($\omega \sim k^z$) at the critical point. The functional dependence on k and ω in Eq. (41) correctly predicts a linear spin wave dispersion $\omega \sim c_s k$ in the symmetry broken state at all temperatures $T < T_c$. On approaching T_c, however, the spin wave spectrum vanishes as the order parameter $\epsilon_k \sim m \sim t^\beta$ where $t = (T_c - T)/T_c$ and β is the appropriate critical exponent. Therefore, exactly at T_c, the spin wave spectrum fades away and above T_c only a delta contribution at $\omega = 0$ survives in the paramagnetic dynamic correlations. Such a description of dynamic critical behavior provided by the approximate form (40) is clearly rather schematic and unsatisfactory. However, the way the spin velocity vanishes $c_s \sim t^\beta$ is consistent with the predictions of dynamic scaling $c_s \sim \xi^{1-z}$ if the dynamic critical exponent is given by $z = d/2$. In fact, by inserting the power law behavior of the correlation length $\xi \sim t^{-\nu}$ near the critical point, we obtain $c_s \sim t^{\nu(d-2)/2}$, which gives $c_s \sim t^\beta$ via standard hyperscaling relations. The latter equality holds because in our approach the correlation exponent $\eta = 0$ due to the analytic k dependence of the correlation functions. Remarkably, the result $z = d/2$ agrees with the general expectations of dynamic scaling for antiferromagnets: The appropriate equation of motion corresponds to "model G" in which the order parameter does not commute with the hamiltonian but a conserved quantity (i.e. the uniform magnetization) is also present[24].

The discussion presented in this Section supports the choice of a simple single mode form as a reasonable approximation of the actual dynamic structure factor in Heisenberg antiferromagnets and leads us to propose Eqs. (37,44) as a closure to the exact renormalization group equation (39), closely following the strategy successfully adopted in classical models[14]. In fact, the thermodynamic relationship (44) between correlations and derivatives of the free energy

holds independently of the form of the interaction $\tilde{w}(\mathbf{k})$ and then it is valid for every Q-system, which corresponds to a potential $\tilde{w}_Q(\mathbf{k})$ characterized by a cut-off Q on its Fourier components. Therefore, the dynamic correlation functions of the Q-systems F_Q^{ij} can be parametrized by the same form (37) used at $Q = d$ with Q-dependent parameters $\mu_{\perp Q}$ and $\mu_{||Q}$ defined by the analog of Eqs. (44):

$$\left(\frac{h_Q}{m}\right)^{-1} = m\left(\frac{\partial a_Q}{\partial m}\right)^{-1} = F_Q^{xx}(\mathbf{g},0) = (\mu_{\perp Q} - 2Jd)^{-1}$$
$$\left(\frac{\partial h_Q}{\partial m}\right)^{-1} = \left(\frac{\partial^2 a_Q}{\partial m^2}\right)^{-1} = F_Q^{zz}(\mathbf{g},0) = (\mu_{||Q} - 2Jd)^{-1} \tag{50}$$

When the *approximate* form (37, 50) of the dynamic correlations is inserted in the *exact* evolution equation (39) we get a *closed* equation for the evolution of the free energy of the Heisenberg model. The frequency sums in Eq. (39) can be analytically evaluated by Euler summation formula while the momentum integration can be trivially carried out with the result:

$$\frac{d\,a_Q}{dQ} = \frac{D_d(Q)}{2\beta}\left\{4\,\ln\left[\frac{\sinh\left(\frac{1}{2}\beta m\mu_{\perp Q}\right)}{\sinh\left(\frac{1}{2}\beta m\sqrt{\mu_{\perp Q}^2 - 4J^2(d^2-Q^2)}\right)}\right] + \ln\left[\frac{\mu_{||Q}^2}{\mu_{||Q}^2 - 4J^2(d^2-Q^2)}\right]\right\} \tag{51}$$

where the "density of states" $D_d(Q)$ is defined as

$$D_d(Q) = \frac{1}{2}\int \frac{d^dk}{(2\pi)^d}\,\delta(\sqrt{d^2-\gamma(\mathbf{k})^2} - Q) \tag{52}$$

This evolution equation will be analyzed in the following Sections.

Finally, it is interesting to consider the limiting form of our equation (51) when $S \to \infty$, i.e. when the quantum Heisenberg model reduces to a classical $O(3)$ vector model. Clearly, we have to rescale all the dimensional quantities by suitable powers of S in order to get a finite result. In particular, the magnetization $m \to Sm$ while energy and temperature must be scaled as $a \to S^2 a$ and $\beta \to S^{-2}\beta$. As a consequence, equation (51) simplifies and we get

$$\frac{d\,a_Q}{dQ} = \frac{D_d(Q)}{2\beta}\left\{2\,\ln\left[\frac{\mu_{\perp Q}^2}{\mu_{\perp Q}^2 - 4J^2(d^2-Q^2)}\right] + \ln\left[\frac{\mu_{||Q}^2}{\mu_{||Q}^2 - 4J^2(d^2-Q^2)}\right]\right\} \tag{53}$$

which in fact coincides with the equation obtained in the framework of HRT for a classical vector model[14].

V. LONG WAVELENGTH ANALYSIS

Let us study the behavior of the QHRT evolution equation (51) in the critical region. This investigation is particularly instructive because it shows how universality and renormalization group (RG) come about in the QHRT framework. We will consider the critical region of the paramagnetic-antiferromagnetic transition, where the physical staggered susceptibilities ($\chi_\perp^s$, $\chi_{||}^s$) diverge. First we remark that our ansatz for the two point function (37) is analytic in $\mathbf{k}$. As a consequence, the correlation exponent predicted by our approach is $\eta = 0$ in any dimension. It is known that such a result is correct only above the upper critical dimension $d = 4$. However, due to the smallness of η in $d = 3$ ($\eta \sim 0.04$[3]), we consider such an approximation acceptable also in the physically relevant applications.

In order to study the critical behavior predicted by our approach, we now focus our attention on the last stages of the evolution ($Q \sim 0$), i.e. on the long wavelength form of equation (51). In fact, we know that the order parameter fluctuations of wavevector $\mathbf{k}$ close to $\mathbf{g}$ are inhibited by the presence of a cut-off Q and the free energy of a Q-system cannot develop singularities at finite Q, but only in the $Q \to 0$ limit. Eqs. (50) show that, in this regime, both $\mu_{\perp Q}$ and $\mu_{||Q}$ tend to $2dJ$. Moreover, being the critical point at $m = 0$, our analysis will be limited to the $m \sim 0$ region. The asymptotic form of the QHRT equation (51) is then:

$$\frac{da_Q}{dQ} = -\frac{\Omega_d}{2\beta(2\pi\sqrt{d})^d}Q^{d-1}\left\{2\ln\left[m^{-1}\frac{\partial a_Q}{\partial m} + J\frac{Q^2}{d}\right] + \ln\left[\frac{\partial^2 a_Q}{\partial m^2} + J\frac{Q^2}{d}\right]\right\} \tag{54}$$

where Ω_d is the surface of the unit d-dimensional hypersphere. Remarkably, this limiting form of the evolution equation coincides with the one appropriate for a classical $O(3)$ vector model in d dimension, i.e. with the long

wavelength limit of Eq. (53). This confirms that Quantum Mechanics becomes irrelevant in the neighborhood of a (finite temperature) critical point[23].

In order to exploit the renormalization group structure hidden in Eq. (54) we suitably rescale the variables:

$$z = \left[\frac{d\,\Omega_d}{2\beta J(2\pi\sqrt{d})^d}\right]^{-1/2} Q^{-(d-2)/2} m$$
$$H = \left[\frac{\Omega_d}{2\beta(2\pi\sqrt{d})^d}\right]^{-1} Q^{-d}[a_Q(m) - a_Q(m=0)] \tag{55}$$

In this way, the explicit dependence of the equation on Q is eliminated and the evolution equation becomes:

$$\dot{H} = dH + z\frac{2-d}{2}H' + \left[\ln\frac{H''+1}{H''(0)+1} + 2\ln\frac{H'/z+1}{H''(0)+1}\right] \tag{56}$$

where dots represent derivatives with respect to $l = \ln(d/Q)$ and primes derivatives in z. This equation is formally identical to that obtained by Nicoll *et al.* in an approximate renormalization group formulation[25] and, as such, it has already been studied by means of standard RG techniques. This analysis showed that the critical point is present only for $d > 2$, in agreement with Mermin-Wagner theorem[17]. Note that precisely at $T = 0$, the QHRT equation (51) does not reduce to the asymptotic form (54) and therefore quantum critical points would require a different long wavelength analysis. Eq. (56) properly embodies critical scaling and hyperscaling and, as shown in Ref.[25], it correctly gives non classical critical exponents to first order in the $\epsilon = 4 - d$ expansion. For instance, the staggered susceptibility exponent at $m = 0$ ($\chi^s_{||} \sim t^{-\gamma}$) is:

$$\gamma = 1 + \frac{5}{22}\epsilon + O(\epsilon^2) \tag{57}$$

The value of γ predicted by our approach in $d = 3$ can be found by integrating the fixed point equation associated to (56) and solving the corresponding eigenvalue problem. The numerical result gives $\gamma = 1.65$, to be compared with the accepted value for a three component order parameter $\gamma = 1.39$[3,26]. The other critical exponents can be obtained from γ by scaling, recalling that $\eta = 0$ in our approximation.

Interestingly, a similar RG analysis can be carried out on the same asymptotic QHRT equation (54) in order to study the divergence of the susceptibility on approaching the *coexistence* curve at $T < T_c$. By rescaling m in the neighborhood of the spontaneous magnetization $m_\times$ as

$$z = \left[\frac{d\,\Omega_d}{2\beta J m_\times(2\pi\sqrt{d})^d}\right]^{-1} Q^{-(d-2)}(m - m_\times)$$
$$H = \left[\frac{\Omega_d}{2\beta(2\pi\sqrt{d})^d}\right]^{-1} Q^{-d}[a_Q(m) - a_Q(m_\times)] \tag{58}$$

the evolution equations at long wavelengths reads:

$$\dot{H} = dH + z(2-d)H' + \left[\ln\frac{H''}{H''(0)} + 2\ln\frac{H'+1}{H'(0)+1}\right] \tag{59}$$

At coexistence, the free energy approaches a fixed point which corresponds to a stationary solution of of Eq. (59), regular in the whole interval $z \in (0, \infty)$ and satisfying the boundary conditions $H(0) = 0$ and $H(z) \to z^{d/(d-2)}$ as $z \to +\infty$. The latter requirement is necessary in order to match with the solution outside the coexistence region (i.e. at $m > m_\times$). As a consequence, the staggered susceptibilities display a non-analytic behavior when $d < 4$:

$$\chi^s_\perp \sim (m - m_\times)^{-2/(d-2)}\,; \qquad \chi^s_{||} \sim (m - m_\times)^{-(4-d)/(d-2)} \tag{60}$$

in agreement with the predictions of a spin wave analysis in the classical $O(3)$ model[3].

Let us conclude this section showing how it is possible to recover, within the QHRT formalism, also the RG equations for the coupling constants of the quantum non linear sigma model ($QNL\sigma M$). The long-wavelength behavior of the d dimensional Heisenberg antiferromagnet in zero external field is commonly believed to be described by a $d+1$ dimensional $QNL\sigma M$, at least in the low temperature regime[27]. This is an effective field theory in which the additional temporal variable, defined only in the interval $(0, \beta)$, reflects the presence of quantum fluctuations. The $QNL\sigma M$ action is conventionally written in terms of a field $\mathbf{\Omega}(\mathbf{r}, t)$ as:

$$S[\mathbf{\Omega}] = \frac{\rho_s}{2} \int d^d\mathbf{r} \int_0^\beta dt \left\{ |\nabla \mathbf{\Omega}|^2 + \frac{1}{c_s^2} \left(\frac{\partial \mathbf{\Omega}}{\partial t} \right)^2 \right\} \tag{61}$$

where the local constraint $|\mathbf{\Omega}| = 1$ is understood and ρ_s and c_s are the bare (i.e. mean field) spin stiffness and velocity. The phase diagram of the model depends on temperature and on the dimensionless coupling constant:

$$g = \frac{c_s \Lambda^{d-1}}{\rho_s} \tag{62}$$

where Λ is the ultraviolet momentum cut-off, which is of the order of the reciprocal of the lattice spacing. The $QNL\sigma M$, as a low energy theory for Heisenberg antiferromagnets, has been extensively studied by Chakravarty Halperin and Nelson (CHN)[9] by weak coupling RG analysis. The one loop equations describing the evolution of the couplings constants are:

$$\begin{aligned} \frac{dg}{dl} &= (1-d)g + \frac{K_d}{2} g^2 \coth(g/2t) \\ \frac{d}{dl}\left(\frac{g}{t}\right) &= -\frac{g}{t} \end{aligned} \tag{63}$$

Here, e^l is the length rescaling factor and K_d is a geometrical coefficient ($K_d^{-1} = 2^{d-1}\pi^{d/2}\Gamma(d/2)$). The equations are written for the running coupling constant $g(l)$ and for the dimensionless temperature scale $t(l)$ whose initial condition is $t = \Lambda^{d-2}/(\beta\rho_s)$. For $d \leq 2$ there are no finite temperature fixed points, while at $T = 0$ and for $d > 1$ there is a non trivial fixed point given by $g_c = 2/K_d(d-1)$ describing a quantum transition. Depending on the initial value of the coupling constant g, the RG flow drives g either to zero or to infinity. In the former case the physics is governed by the low temperature fixed point and then the system is ordered. Assuming that the two dimensional Heisenberg model has a symmetry breaking ground state, from the solution of the RG equations (63), the following behavior of the correlation length is obtained[9]:

$$\xi(T) \sim \xi_0 \mathrm{e}^{\frac{2\pi\bar{\rho}_s}{T}} \tag{64}$$

where $\bar{\rho}_s = \rho_s(g_c - g)/g_c$ is the renormalized spin-stiffness at $T = 0$.

The weak coupling RG analysis predicts several regimes where quantum and thermal fluctuations play different roles. However, quantitative estimates based on low energy effective theories are usually rather inaccurate because short wavelength fluctuations are neglected in these approaches. Here we want to show that the QHRT equation, reduces, at low energy, precisely to the one loop RG equations studied by CHN (63). However, QHRT provides a description of spin fluctuations over *all* lengthscales maintaining the advantages of a fully microscopic theory.

In the low temperature region, longitudinal fluctuations can be neglected because they are characterized by a less singular behavior and therefore, in this regime, the last term in Eq. (51) may be dropped. If we now differentiate Eq. (51) with respect to the magnetization, we get an equation for the evolution of the staggered field $h_Q(m)$ at fixed m:

$$\begin{aligned} \frac{dh_Q}{dQ} = D_d(Q) \Bigg[& \coth\left(\frac{\beta}{2} m \mu_{\perp Q}\right) \mu_{||Q} \\ & - \coth\left(\frac{\beta m}{2}\sqrt{\mu_{\perp Q}^2 - 4J^2(d^2-Q^2)}\right) \frac{\mu_{\perp Q}\mu_{||Q} - 4J^2(d^2-Q^2)}{\sqrt{\mu_{\perp Q}^2 - 4J^2(d^2-Q^2)}} \Bigg] \end{aligned} \tag{65}$$

This equation implicitly describes how the spontaneous magnetization is reduced from its mean field estimate when fluctuation are included. In order to exploit this information, it is useful to define a Q-dependent spontaneous magnetization m_Q by requiring that $h_Q(m_Q) = 0$. Such a quantity satisfies an evolution equation which can be easily deduced from Eq. (65). At long wavelengths (i.e. keeping the leading terms as $Q \to 0$) the Q dependent staggered magnetization in zero field obeys a closed equation:

$$\frac{dm_Q}{dQ} = K_d \left(\frac{Q}{\sqrt{d}}\right)^{d-2} \coth(\beta Q m_Q) \tag{66}$$

In order to make contact with the RG picture based on the $QNL\sigma M$ effective action, we now have to relate the QHRT variable m_Q with the running coupling constant $g(l)$ appearing in Eqs. (63). The correspondence between the length rescaling factors is clearly $l = \ln(d/Q)$, while the definition of the coupling constant g in terms of physical

quantities, like stiffness and spin velocity, given in Eq. (62) suggests the proportionality between g^{-1} and the spontaneous magnetization. In fact, as discussed in Section (IV), QHRT provides explicit relations between ρ_s, c_s and the magnetization at coexistence. It is therefore rather natural to introduce an "effective coupling constant" $g_Q = \sqrt{4d}(Q/\sqrt{d})^{d-1} m_Q^{-1}$ which, when substituted in Eq. (66), satisfies an equation formally identical (to order g^2) with the standard one loop RG form (63). As an example, we plot in Figure [1] the RG flux of g_Q as obtained by the integration of the *full* QHRT equation in $d = 2$ (51) via the previous definition of g_Q. We clearly see the effect of the unstable zero temperature weak coupling fixed point while, for the nearest neighbor Heisenberg model, the other fixed point ($g_c = 4\pi$), governing the Quantum Critical regime, has no effect on the RG trajectories. This suggests that the Heisenberg model always remains in the Renormalized Classical regime in agreement with an independent analysis based on the pure quantum self consistent harmonic approximation (PQSCHA)[12].

VI. NUMERICAL RESULTS

Equation (51), together with the thermodynamically consistent closure relations (50) and the appropriate initial condition at $Q = d$ (34) has been solved numerically in two and three dimensions and several values of the spin S. Following the analogous treatment of HRT in classical systems[14] we first wrote the partial differential equation in quasilinear form and then used a fully implicit finite difference scheme[28]. A careful implementation of the numerical algorithm is necessary, because the solution to the QHRT equation develops singularities as $Q \to 0$, when a phase boundary is crossed. This is a consequence of the special treatment of long wavelength fluctuations provided by QHRT which is able to reproduce rigorously flat isotherms inside the coexistence region, as already shown in classical systems[29]. Our computations were carried out with a mesh of few hundred points along the magnetization axis, which already allows for a good accuracy. The high temperature asymptotic behavior of thermodynamic quantities is correctly reproduced by QHRT in arbitrary dimension d and for every spin S, as can be easily shown by analysis of the evolution equation (51). Before discussing the numerical results in three dimensions we briefly comment on the calculations performed on the square lattice. In this Section we set $J = 1$.

A. The two dimensional case

As already noticed, our equation correctly predicts the absence of spontaneous symmetry breaking at finite temperature for every choice of the spin S. However, the effective coupling constant flow shown in Fig. [1] illustrates the strong attractive nature of the unstable zero temperature fixed point and allows to give a precise estimate of the ground state spontaneous magnetization. For $S = 1/2$ we obtain $m_\times \sim 0.35$, rather close to the value $m \sim 0.307$ obtained by numerical simulations[7]. Weak coupling RG analysis predicts that the correlation length at $m = 0$ diverges exponentially on approaching zero temperature with a coefficient related to the spin stiffness (64). The same behavior is found by our numerical results as shown in Fig. [2]. This result is not unexpected because we have already shown that QHRT contains all the information provided by the one loop RG approach. The estimate of the spin stiffness coming from a linear fit of the data in Fig. [2] gives $\rho_s \sim 0.12$ for $S = 1/2$, to be compared with the accepted value $\rho_s \sim 0.18$[7]. Our result is in fact consistent with the relationship $\rho_s = m_\times^2$ discussed in Section (IV) which follows from the adopted closure. Therefore we are led to conclude that the discrepancy between the QHRT and Monte Carlo (MC) in the estimated values of ρ_s is probably due to the crude approximation for the two point functions we have adopted in this calculation, as anticipated in Section (IV), see also Eq. (49).

The zero field specific heat C_H as a function of temperature is shown in Fig. [3] together with a comparison with MC data for $S = 1/2$[30]. The non monotonic behavior, even in the absence of a phase transition, is just a consequence of the asymptotic decay of C_H at high temperature ($C_H \propto T^{-2}$) and to the vanishing of C_H at $T = 0$, as required by thermodynamics.

B. The Heisenberg model on a cubic lattice

In $d = 3$, spontaneous symmetry breaking at finite temperature does occur in the Heisenberg model. As a consequence, thermodynamics forces the Helmholtz free energy to be rigorously flat inside the coexistence region. This feature is usually lost in the approximate treatments of the model and may be recovered *a posteriori* by Maxwell double tangent construction. As already noticed in the application of HRT to classical statistical models, our approach instead is able to predict rigorously flat isotherms in a region of the phase diagram, thereby allowing for a unambiguous determination of the coexistence curve[29]. As an example, in Fig. [4] we show the behavior of the equation of state $h(m)$

at two temperatures: above and below T_c for several values of the evolution parameter Q. We see that, although the initial condition at $Q = 3$ is in both cases below the mean field critical temperature (i.e. corresponding to a negative mean field transverse susceptibility), $\chi_\perp^{-1} = h/m$ is strongly renormalized by fluctuations and for $T > T_c$ it becomes positive and saturates as $Q \to 0$, while for $T < T_c$ eventually sticks to zero. Therefore, during the evolution, the region characterized by negative susceptibility is gradually removed (for $T > T_c$) or replaced by a flat isotherm (for $T < T_c$). This behavior can be analytically understood from a study of the asymptotic equation, in close analogy to the Ising case[29].

The full coexistence curve for $S = 1/2$ and $S = \infty$ is reported in Fig. [5] together with the results of series expansions[5] and numerical simulations[2]. The zero temperature limit of the spontaneous magnetization gives $m_\times = 0.43$ in our approximation, to be compared with the value 0.42 from second order spin-waves theory[6]. The predicted critical temperature is shown in Table I for several values of the spin S. When available, also estimates from Monte Carlo, series expansions or cumulant expansions are given. In Fig. [6] the specific heat as a function of the temperature is plotted for $S = 1/2$ and $S = \infty$ together with classical MC simulations and recent QMC data[4]. Note that QHRT correctly reproduces the different zero temperature limit of the quantum ($C_H \to 0$) and classical ($C_H \to NJ$) systems. Again, the agreement is quite satisfactory, being comparable with simulation uncertainties. We remark that QHRT correctly predicts a cusp-like behavior at T_c, although the corresponding critical exponent $\alpha < 0$ is underestimated by our approximation. These small differences, however, cannot be appreciated on the scale of the plot. Finally, Fig. [7] shows the change in the shape of the coexistence curve due to the effects of quantum fluctuations: going from the classical ($S = \infty$) to the quantum $S = 1/2$) case, the magnetization curve rounds off and the linear behavior at low temperature disappears, in agreement with SWT which predicts a quadratic temperature dependence of $m_\times$ as $T \to 0$.

In summary, we believe that even within the crude simple pole approximation adopted in the present study, QHRT is able to get quantitative agreement with recent numerical data on the thermodynamics of quantum antiferromagnets in $d = 3$. The error can be estimated in few percents on the critical temperature, spontaneous magnetization and specific heat. Larger discrepancies can be seen in the shape of the coexistence curve: such a disagreement is rather unexpected and more accurate simulation data are needed before reaching a definite conclusion on this delicate issue.

VII. CONCLUSIONS

In this paper we have introduced a new theoretical tool for the study of phase transitions in quantum systems. Such an approach is based on the use of the Hierarchical Reference Theory (HRT)[14], a theory developed in the context of classical fluids able to correctly describe the system in a wide region of the phase diagram, both near and far from the critical point. Fluctuations over different lengthscales are gradually included thereby reproducing the full structure of Wilson renormalization group theory in the critical region. The possibility of applying HRT also in the context of quantum systems (QHRT) follows from the observation that the grand partition function of a wide class of quantum models can be formally mapped onto a classical partition function (in $d+1$ dimensions) to which HRT can be directly applied. The advantage of our formulation is that since this mapping is exact, the microscopic informations are correctly included into this formalism and only in the vicinity of the critical point and at long wavelengths the peculiar features of the model disappear and the evolution equations acquire a universal form. QHRT is a general approach which can in principle be applied to a large class of systems including fermions, bosons and spins.

The validity of this theory has been studied in the specific case of the isotropic Heisenberg antiferromagnet. This choice is dictated by the large amount of available results from other theories and numerical methods, which include mean field theories[18], renormalization group[9] and path integral approaches[12], series expansions[5] or Quantum Monte Carlo simulations[4]. In order to obtain a closed and tractable equation out of the QHRT formalism, we analyzed a simple approximation which amounts to parameterize the dynamic correlations in a single pole form. Even within this approximation scaling and hyperscaling are satisfied close to the critical point, the critical exponents are correct near four dimensions and, in $d = 3$, take non classical values slightly larger than the accepted ones. Remarkably, the weak coupling renormalization group equations for the Non Linear Sigma Model are recovered at low temperature even in $d = 2$, thereby reproducing the correct asymptotic scaling as $T \to 0$.

The theory has been tested against numerical data on a simple cubic lattice with nearest neighbors interaction and for several values of the spin. The results are in close agreement with available simulations for several quantities like the location of the critical point, the spontaneous magnetization and the specific heat. In $d = 2$ the comparison with simulations is less satisfactory even if QHRT is able to reproduce the qualitative behavior of the model. The discrepancies we found are related to the single mode approximation adopted in the closure of the equation and may be overcome by use of a more flexible form for the dynamic structure factors.

In this paper our attention has been focused on the Heisenberg model since it allows for several interesting gen-

eralizations, like the introduction of anisotropies or competing interactions. In these cases, quantum and thermal fluctuations may play a more fundamental role in modifying the topology of the phase diagram. A detailed study of the Heisenberg model with easy plane anisotropy is under way: the results will shed light on the thermodynamics of the crossover between two and three component order parameter, with direct experimental implications. An extremely interesting application of the QHRT formalism to fermionic systems regards the Hubbard model, whose hamiltonian has in fact the general structure of Eq. (1). The natural choice, as a reference system, is the free Fermi gas on the lattice in an external magnetic field, while the Hubbard interaction couples the on site electron densities. In this case, the evolution equations will involve density and magnetization fluctuations allowing for a characterization of the phase transitions which lead to the creation of magnetic structures (ferro, antiferro or itinerant) or charge density wave instabilities (phase separation or stripe formation). We believe that a theory able to deal with long wavelength fluctuations, like QHRT, may represent a useful tool for tackling this class of problems.

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	QHRT	Monte Carlo	Series
$S = 1/2$	0.90	0.94[4]	0.93[5]
$S = 1$	2.66		
$S = 3/2$	5.16		
$S = 2$	8.35		
$S = 5/2$	12.25		
$S = \infty$	1.419	1.443[26]	1.445[1]

TABLE I. *Critical temperatures for different values of the spin obtained by QHRT and other methods in the three dimensional Heisenberg model.*

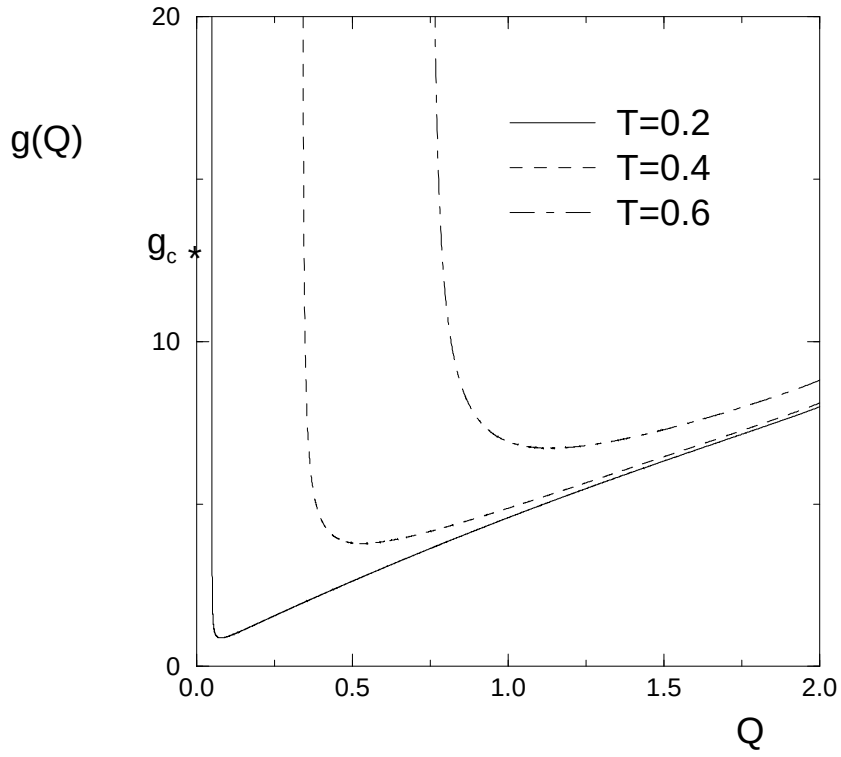

FIG. 1. *RG trajectories for the two dimensional Heisenberg model computed via numerical integration of the QHRT equation.*

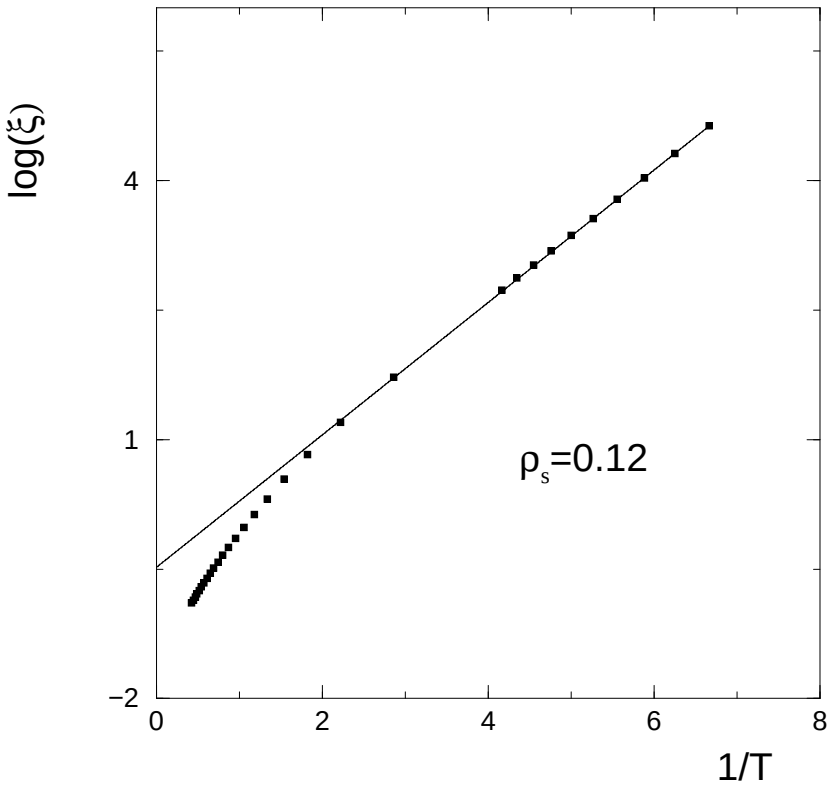

FIG. 2. *Correlation length in two dimensions for* $S = 1/2$.

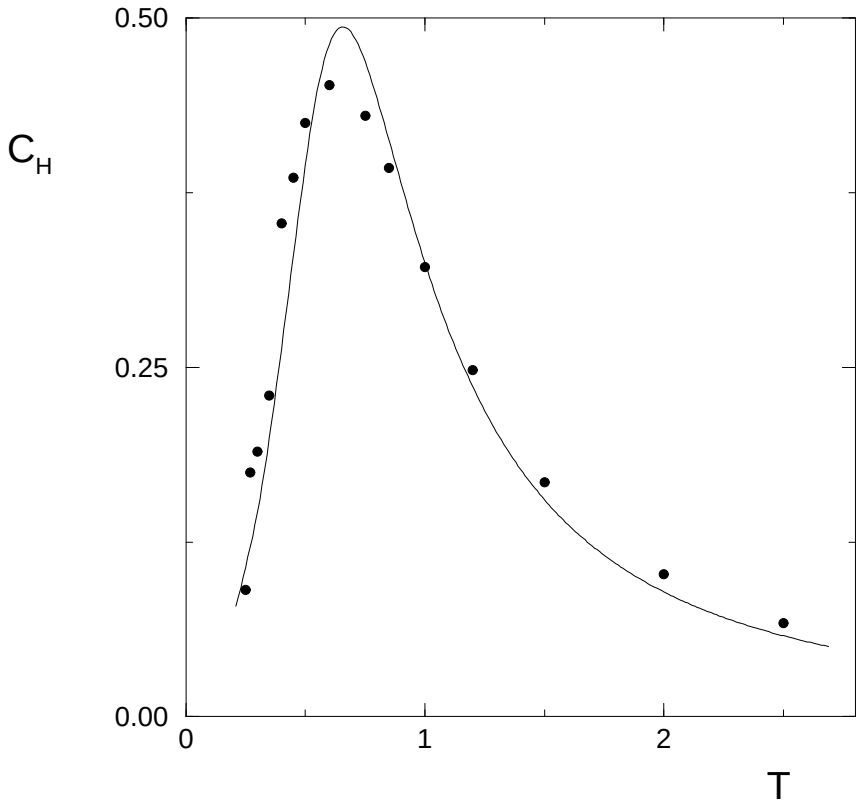

FIG. 3. *Zero field specific heat C_H as a function of temperature for the $S = 1/2$ case in two dimensions. Full line QHRT, circles Monte Carlo simulations*[30].

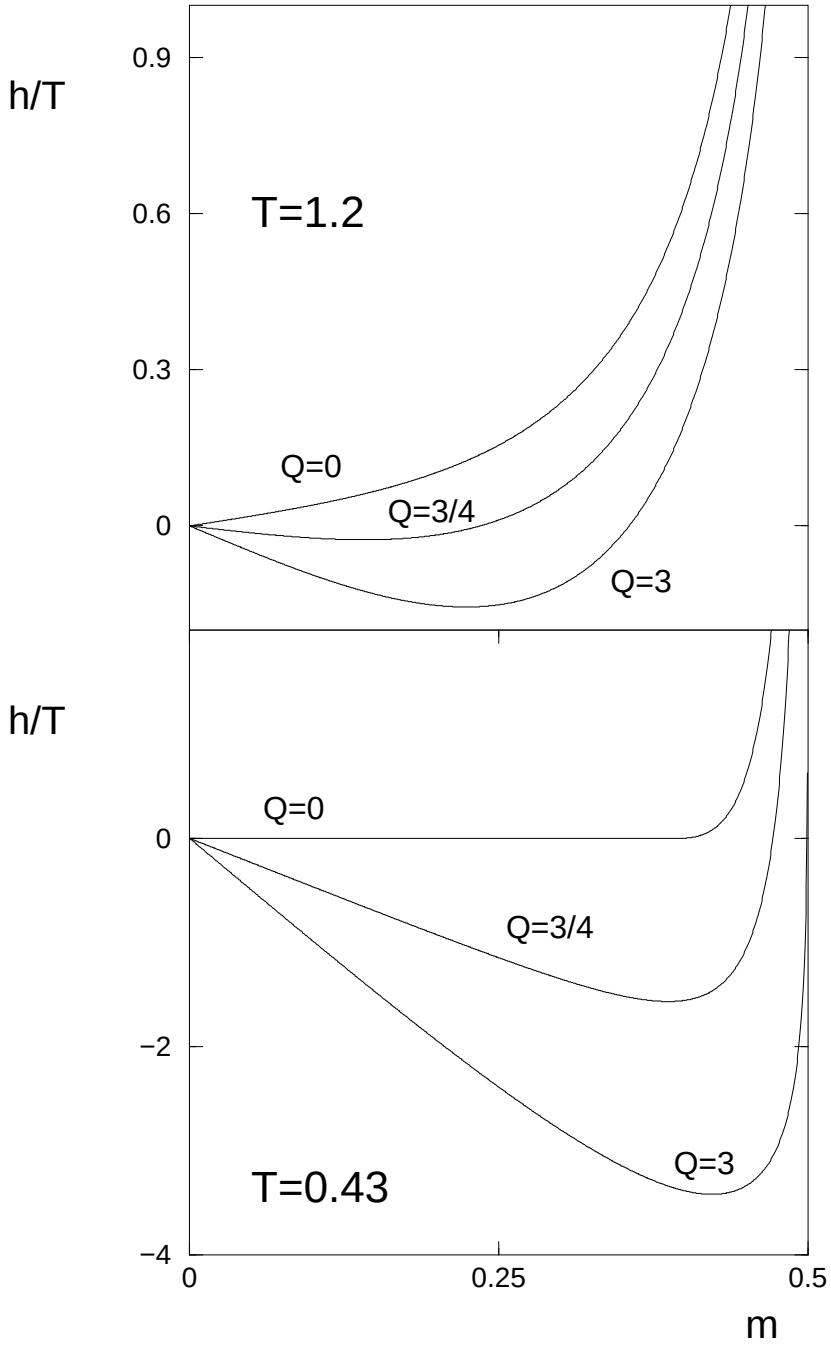

FIG. 4. *Behavior of the equation of state $h(m)$ at two different temperatures as a function of the evolution parameter Q. Above $T_c < T = 1.2 < T_{\rm MF} = 1.5$, being $T_{\rm MF}$ the critical temperature in Mean-Field approximation. Below $T = 0.43 < T_c$.*

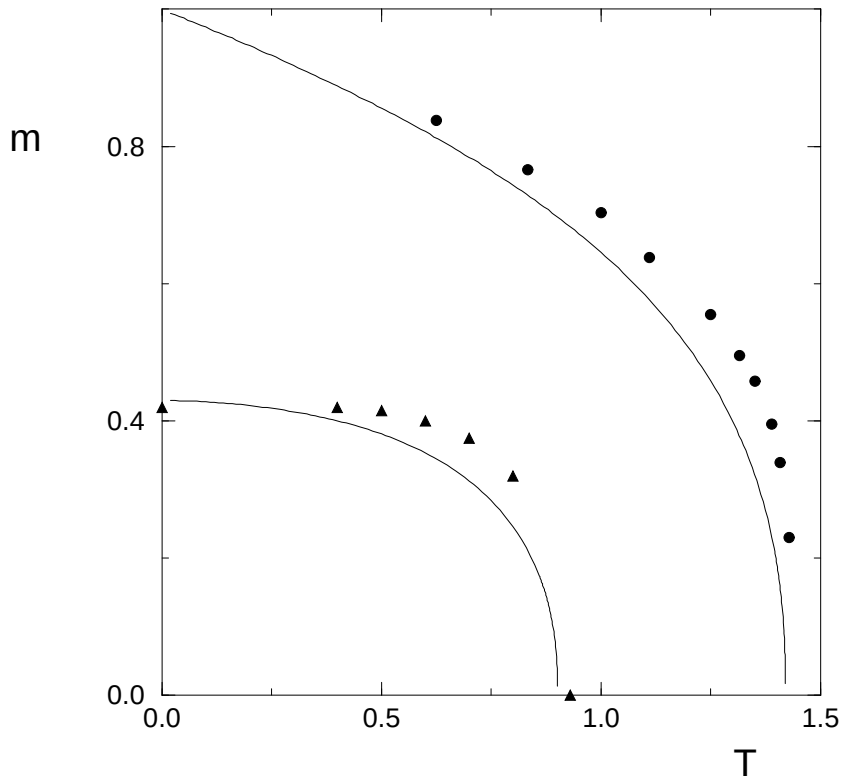

FIG. 5. *Above: Coexistence curve of the classical Heisenberg model. Full line QHRT, circles Monte Carlo simulations*[2]. *Below: Coexistence curve of the* $S = 1/2$ *Heisenberg model. Full line QHRT, triangles series expansion*[5].

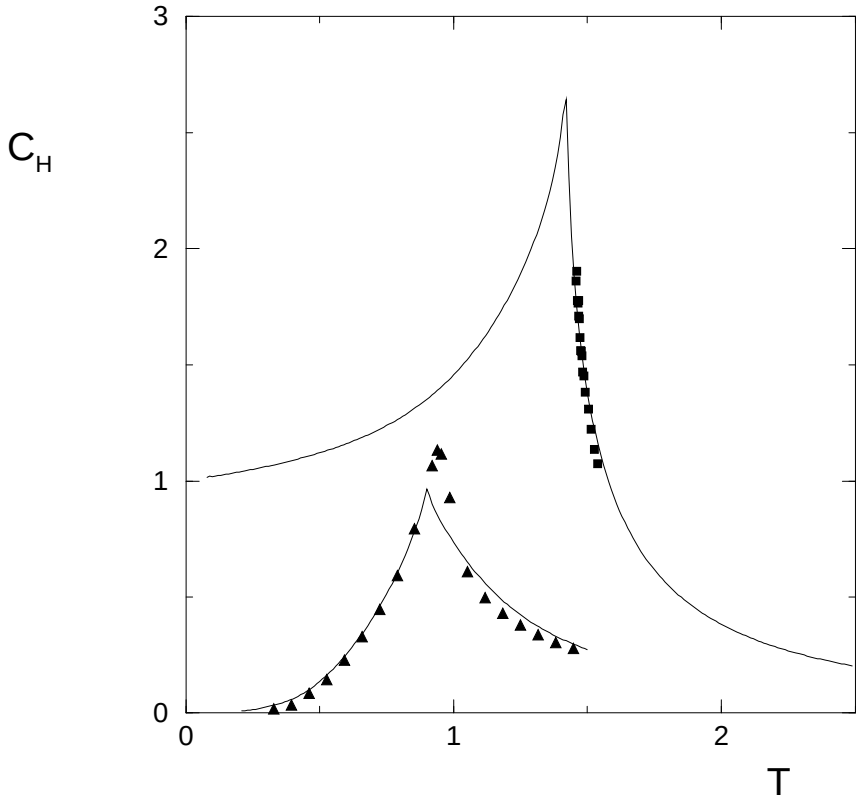

FIG. 6. *Above: Specific heat of the classical Heisenberg model. Full line QHRT, squares Monte Carlo simulation*[31]*. Below: Specific heat of the* $S = 1/2$ *Heisenberg model. Full line QHRT, triangles Monte Carlo simulations*[4]*.*

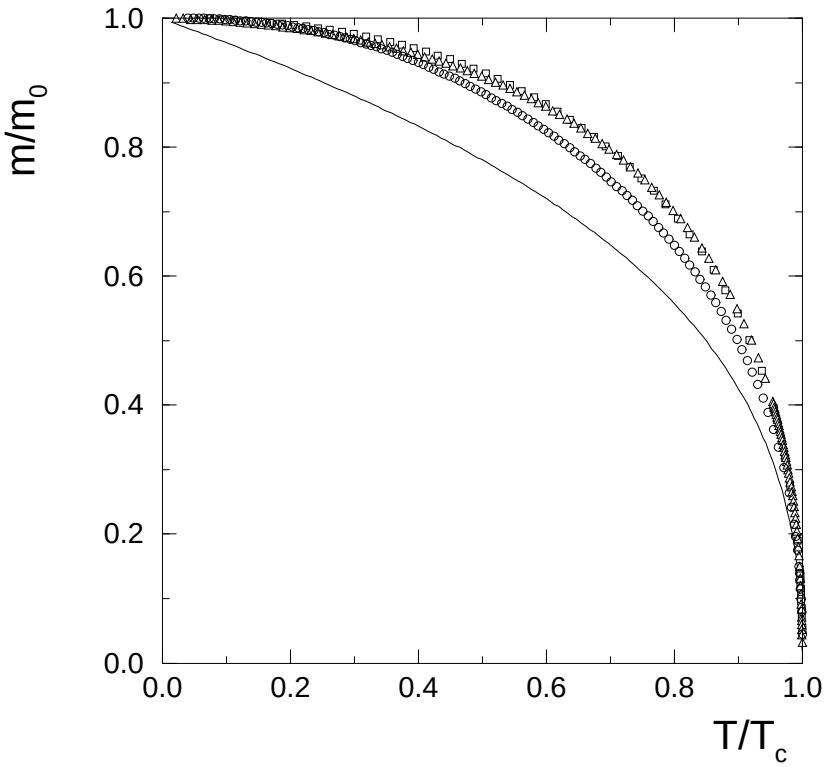

FIG. 7. *Reduced spontaneous magnetization as a function of temperature for different values of the spin:* $S = 1/2$ *(triangles)* $S = 1$ *(squares)* $S = 5/2$ *(circles) and* $S = \infty$ *(full line).*